The Analytical Information Markup Language Project

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Folks, we got TROUBLE, right here in Science City. It starts with T, and it rhymes with D, and it stands for DATA…

- Can't move it
  - From instrument to instrument
  - From instrument to application
  - From application to application
- Can't interconvert it
- Can't find all its parts
- Can't look at it easily
- Can't use it easily with modern computing and networking technologies

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There is crisis in archiving and retrieving data

- We're drowning in data, yet increasingly we cannot find our stuff because of
  - Incredible Success of Hyphenated and Multiplexed Analytical Techniques
  - Moore's Law
- Data mining can increase the value of archived data, but…
- Regulatory agencies are now demanding extraordinarily long data retention
- In terms of retrieving archived data, we were better off with paper forty years ago before the arrival of lab computers…
- We can still read the data in Newton's notebooks today; will folks be able to read ours in 100, 20, or even 5 years?

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What Are the AnIML Standards?

- The AnIML Standards are projects of ASTM Committee E13 on Spectroscopy and Separation Science, Subcommittee E13.15 on Analytical Data

- AnIML is a markup language based on Extensible Markup Language (XML)

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The Analytical Information Markup Language (AnIML)

- has been developed expressly for analytical chemistry result data and metadata
- defines a data format for representing all types of result data and metadata
- provides a system for identifying content (data elements and attributes) with labels (tags)
- provides a model and the means for defining the structure, content, and semantics of result data and metadata in documents
- expresses shared vocabularies
- allows machines to carry out rules made by people

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AnIML Components

- AnIML Core Schema
  - One Schema
  - Maintained by ASTM E13.15
- AnIML Technique Schema
  - One Schema
  - Maintained by ASTM E13.15
- AnIML Technique Definition Documents
  - One or More Instance Documents per Technique
  - Maintained by ASTM E13 or Appropriate Domain Expert Organization
- AnIML Technique Definition Extensions
  - One Instance Document per Technique Created from the Appropriate Base Technique Definition
  - Maintained by Vendor, Organization, User, or Whomever Extends the Technique
- AnIML Result Data Files

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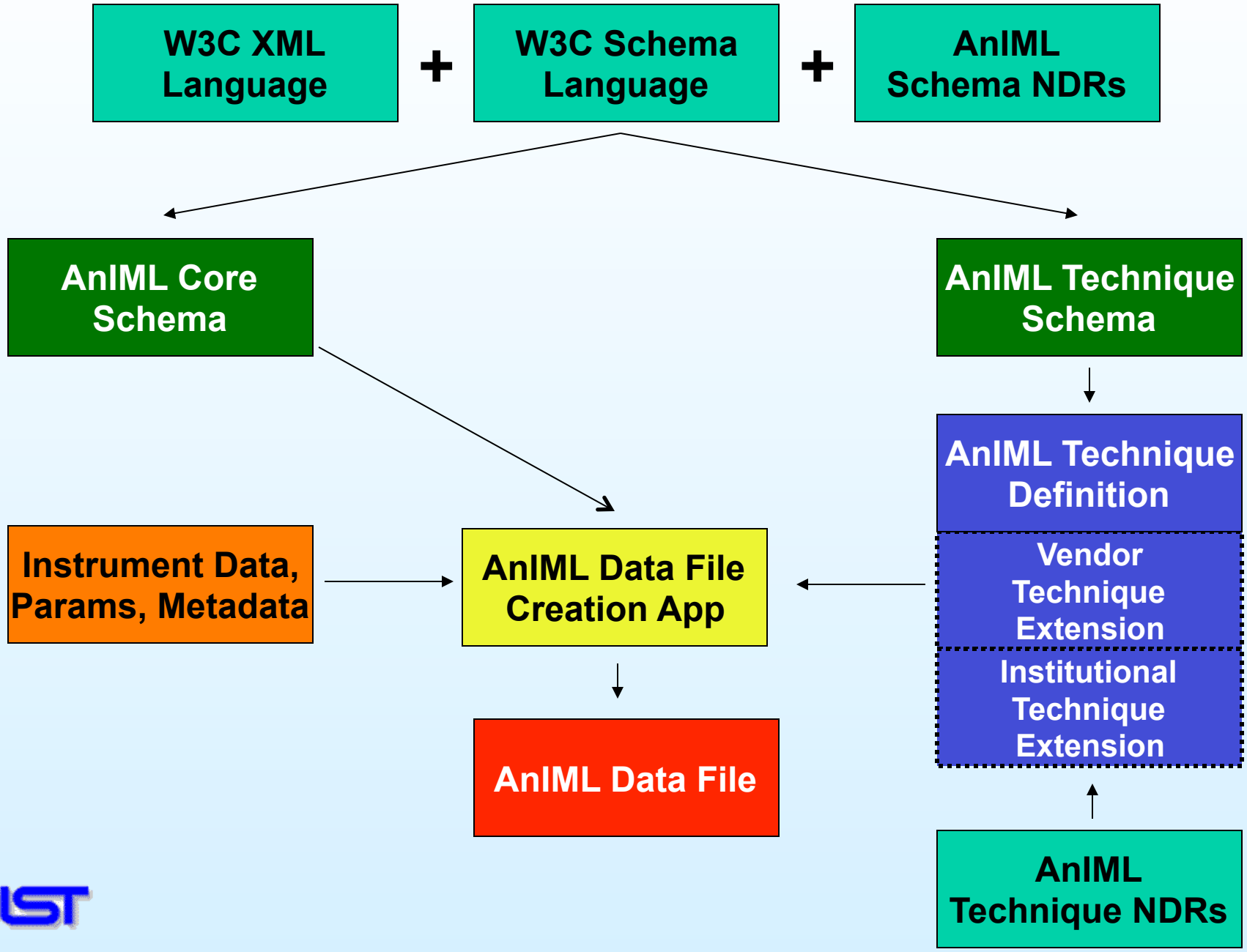
Basis for Creating an AnIML Data File



Some AnIML Files are Simple

Some AnIML Files are Complex

Key Features of AnIML

- Extensible
- Can Accommodate ANY Type of Data
- Verifiable Using Digital Signatures
- Traceable through Audit Trails
- Validateable Against Data Format Rules, Data Structure Rules, & other Data Requisites

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AnIML: Where We're At for Version 1.0

- AnIML Core Schema
  - Complete
  - Frozen
  - Internally Documented
- AnIML Schema NDRs
  - Complete
- AnIML Technique Schema
  - Complete
  - Frozen
  - Internally Documented
- AnIML Technique NDRs
  - In Progress
- AnIML Technique Exemplar
  - In Progress

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AnIML: Where We're At for Version 1.0

- AnIML Technique Definitions
  - UV-Vis Technique Definition – Complete
  - Chromatography Technique Definition – Complete
  - Mass Spec Technique Definition – Started
  - 1D NMR Technique Definition – Started
  - IR Technique Definition – Started
  - Point Detector Technique Definitions
    - GC Detectors (5) – Complete
    - LC Detectors – Started
  - AnIML Misc. Technique Definitions
    - Indexing – Complete
    - Cross-Cutting – Not Started
    - Trace Forming – Not Started
    - Peak Table – Not Started

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AnIML: Where We're At for Version 1.0

- AnIML Applications and Tools
  - AnIML Data Viewers – Several Complete
  - AnIML Extensible Validator – Complete
  - Simple AnIML File Writer for Agilent 8453 UV/Vis – Complete
  - JCAMP-DX to AnIML Data Converters – Several Complete
  - XSLT Documentation Extractor for Schemas – Complete
  - Documentation Extractor for Technique Definitions – Complete

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AnIML Documents and Standards

- AnIML Standard Practice Document – Nearly Complete
- AnIML Core and Technique Schema Standard Specification and Guide Document
- AnIML Standard Technique Definition Guide Document
- Individual Technique Standard Specification and Guide Documents
  - AnIML UV-Vis Technique
  - AnIML IR Technique
  - AnIML Chromatography Technique
  - AnIML Mass Spec Technique
  - AnIML 1D NMR
  - AnIML Misc. Techniques
    - Indexing
    - Point Detectors
    - Cross-Cutting
    - Trace Forming
    - Peak Table

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Expediting the Completion of AnIML 1.0

- Current volunteer effort is too slow
- There is still too much to do
- Need paid help to develop components and documentation
- AnIML 1.0 Documentation Expedition Project
  - Funded by
    - Agilent Technologies
    - Amgen
    - Glaxo SmithKline
    - PerkinElmer
    - Waters Corporation
  - Administered by ASTM

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Want to Know More about AnIML?

- AnIMLWebsite
  - http://animl.sourceforge.net
  - http://www.animl.org
- PittCon 2012
  - SEDD & AnIML Networking Session - Monday AM
  - AnIML Workshop – Thursday PM
- SLAS 2012
  - 2:00 PM Today Room 1AB Burkhard Schäfer
  - BSSN White Paper

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Want to Help Develop AnIML?

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  - bschaefer@bssn-software.com
- Webex Virtual Meetings
  - Monthly – 10:30 AM EST
  - ASTM-sponsored

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